# On the test of the modified BCS at finite temperature

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## Abstract

The results and conclusions by Ponomarev and Vdovin [Phys. Rev. C **72**, 034309 (2005)] are inadequate to judge the applicability of the modified BCS because they were obtained either in the temperature region, where the use of zero-temperature single-particle spectra is no longer justified, or in too limited configuration spaces.

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The modified BCS theory (MBCS) was proposed and developed in [1, 2, 3] as a microscopic approach to take into account fluctuations of quasiparticle numbers, which the BCS theory neglects. The use of the MBCS in nuclei at finite temperature $T$ washes out the sharp superfluid-normal phase transition. This agrees with the predictions by the macroscopic theory [4], the exact solutions [5], and experimental data [6]. The authors of [7] claimed that the MBCS is thermodynamically inconsistent and its applicability is far below the temperature where the conventional BCS gap collapses. The present Comment points out the shortcomings of [7]. We concentrate only on the major issues without repeating minor arguments already discussed in [2, 3] or inconsistent comparisons in Fig. 9 and footnote [11] of [7] (See [8]).

1) The application of the statistical formalism in finite nuclei requires that $T$ should be small compared to the major-shell spacings ($\sim$ 5 MeV for $^{120}$Sn). In this case zero-$T$ single-particle energies can be extended to $T \neq 0$. As a matter of fact, the $T$-dependent Hartree-Fock (HF) calculations for heavy nuclei in [9] have shown that already at $T \geq 4$ MeV the effect of $T$ on single-particle energies cannot be neglected. We carried out a test calculation of the neutron pairing gap for $^{120}$Sn, where, to qualitatively mimic the compression of the single-particle spectrum at high $T$ as in [9], the neutron energies are $\epsilon_j' = \epsilon_j(1+\gamma T^2)$ with $\gamma = -1.2 \times 10^{-4}$ if $|j\rangle \leq |1g_{9/2}\rangle$. For $|j\rangle$ above $|1g_{9/2}\rangle$, we took $\gamma$ equal to $0.49 \times 10^{-3}$ and $-0.7 \times 10^{-3}$ for negative and positive $\epsilon_j$, respectively. The obtained MBCS gap has a smooth and positive $T$ dependence similar to the solid line in Fig. 7 of [1] with a flat tail of around 0.2 MeV from $T = 5$ MeV up to $T = 7$ MeV. For the limited spectrum used in the calculations of Ni isotopes [2], the major-shell spacing between (28-50) and (50-82) shells is about 3.6 MeV, so the region of valid temperature is $T \ll 3.6$ MeV. Hence, the strange behaviors in the results obtained at large $T$ for $^{120}$Sn and Ni isotopes in [7] occurred because the zero-$T$ spectra were extended to too high $T$. Moreover, the configuration spaces used for Ni isotopes are too small for the MBCS to be applied at large $T$. The same situation takes place within the picket-fence model (PFM) analyzed below.

2) The virtue of the PFM is that it can be solved exactly in principle at $T = 0$. However, at $T \neq 0$ the exact solutions of a system with pure pairing do not represent a fully thermalized system. As a result, temperatures defined in different ways do not agree [10]. The limitation of the configuration space with $\Omega = 10$ causes a decrease of the heat capacity $C$ at $T_{\rm M} > 1.2$ MeV(Schottky anomaly) [3] (See Fig. 4 (c) of [7]). Therefore, the region of $T > 1.2$ MeV,

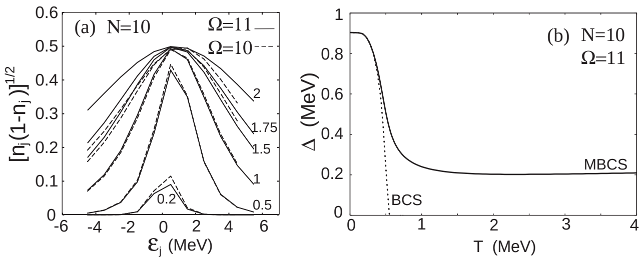


FIG. 1: (a) MBCS quasiparticle-number fluctuations $\delta\mathcal{N}_j$ within the PFM versus single-particle energies at several $T$. Lines connect discrete values to guide the eyes; numbers at the lines show the values of $T$ in MeV; (b) BCS and MBCS gaps for $N = 10$ and $\Omega = 11$ ($G = 0.4$ MeV).

generally speaking, is thermodynamically unphysical. The most crucial point here, however, is that such limited space deteriorates the criterion of applicability of the MBCS (See Sec. IV. A. 1 of [3]), which in fact requires that the line shapes of the quasiparticle-number fluctuations $\delta\mathcal{N}_j \equiv \sqrt{n_j(1-n_j)}$ should be included symmetrically related to the Fermi level [Fig. 1 (f) of [3] is a good example]. The dashed lines in Fig. 1 (a) shows that, for $N =$ 10 particles and $\Omega = 10$ levels ($G = 0.4$ MeV), at $T$ close to 1.78 MeV, where the MBCS breaks down, $\delta\mathcal{N}_j$ are strongly asymmetric and large even for lowest and highest levels. At the same time, by just adding one more valence level ($\Omega = 11$) and keeping the same $N =$ 10 particles, we found that $\delta\mathcal{N}_j$ are rather symmetric related to the Fermi level up to much higher $T$ [solid lines in Fig. 1 (a)]. This restores the balance in the summation of partial gaps $\delta\Delta_j$ [3]. As a result the obtained MBCS gap has no singularity at $0 \leq T \leq 4$ MeV [Fig. 1 (b)]. The total energy and heat capacity obtained within the MBCS also agree better with the exact results than those given by the BCS [Fig. 2]. It is worth noticing that, even for such small $N$, adding one valence level increases the excitation energy $E^*$ by only $\sim 10\%$ at $T = 2$ MeV, while at $T < 2$ MeV the values of $E^*$ for $\Omega = 10$ and 11 are very close to each other. We also carried out the calculations for larger particle numbers $N$. This eventually increases $T_{\rm M}$, and also makes the line shapes of $\delta\mathcal{N}_j$ very symmetric at much higher $T$. For $\Omega = 50$ and 100, e.g., we found $T_{\rm M} > 5$ MeV, and the MBCS gap has qualitatively the same behavior as that of the solid line in Fig. 1 (b) up to $T \sim 5$ - 6 MeV. However, for large $N$ the exact solutions of PFM turn out to be impractical as a testing tool for $T \neq 0$. Since all the exact eigenstates must be included in the partition function $Z$, and, since for $N = 50$ e.g., the number of zero-seniority states alone already reaches $10^{14}$, the calculation of exact

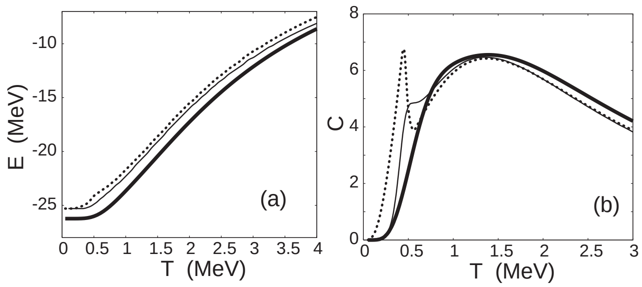


FIG. 2: Total energies (a) and heat capacities (b) within the PFM for ($N$ = 10, $\Omega$ = 11, $G$ = 0.4 MeV) versus $T$. Dotted, thin-, and thick-solid lines denote the BCS, MBCS and exact results, respectively. A quantity equivalent to the self-energy term $-G\sum_j v_j^4$, not included within BCS and MBCS, has been subtracted from the exact total energy.

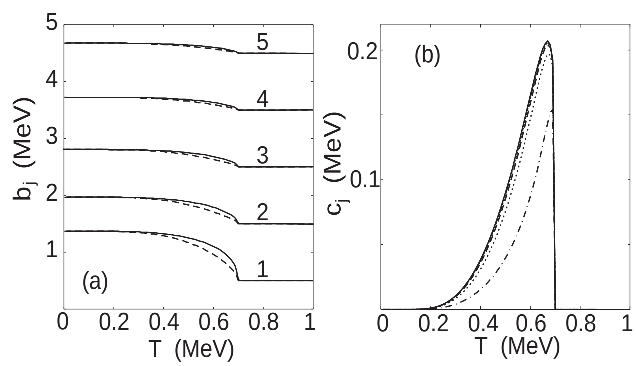


FIG. 3: $b_j$ (a) and $c_j$ (b), obtained within BCS for 5 lowest levels in the PFM with $\Omega = 10$ versus $T$. In (a) the solid and dashed lines represent $b_j$ and quasiparticle energies $E_j$, respectively. In (b) the solid, dashed, dotted, and dash-dotted lines correspond to levels $1-5$ in (a), respectively.

$Z$ becomes practically impossible.

3) The principle of compensation of dangerous diagrams was postulated to define the coefficients $u_j$ and $v_j$ of the Bogoliubov canonical transformation. This postulation and the variational calculation of $\partial H'/\partial v_j$ lead to Eq. (19) in [7] for the BCS at $T = 0$. It is justified so long as divergences can be removed from the perturbation expansion of the ground-state energy. However, at $T \neq 0$ a $T$-dependent ground state does not exist. Instead, one should use the expectation values over the canonical or grand-canonical ensemble [2, 3]. Therefore, Eq. (19) of [7] no longer holds at $T \neq 0$ since the BCS gap is now defined by Eq. (7) of [7], instead of Eq. (3). Fig. 3 clearly shows how $b_j \neq E_j$ and $c_j \neq 0$ at $T \neq 0$. This invalidates the critics based on Eq. (19) of [7].

In conclusion, the test of [7] is inadequate to judge the MBCS applicability because its results were obtained either in the $T$ region, where the use of zero-$T$ spectra is no longer valid (for $^{120}$Sn and Ni), or within too limited configuration spaces (the PFM for $N = \Omega = 10$ or 2 major shells for Ni). Our calculations with a $T$-dependent spectrum for $^{120}$Sn, and within extended configuration spaces presented here show that the MBCS is a good approximation up to high $T$ even for a system with $N = 10$ particles.

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